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1,2-Bis(3-phenoxybenzylidene)hydrazine

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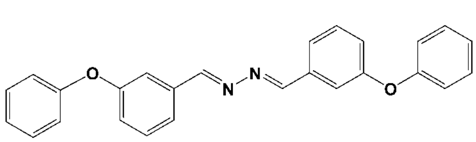
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.144; data-to-parameter ratio = 17.2.

Molecules of the title compound, $C_{26}H_{20}N_2O_2$, reside on crystallographic centres of inversion located at the mid-point of the N—N bond. The benzylidene ring is essentially coplanar with the central hydrazine group, with an interplanar angle of 4.5 (2)°, whereas the phenyl ring is oriented at 34.0 (3)° with respect to the mean plane of the central 1,2-dibenzylidenehydrazine group. In the crystal, C—H$\cdots\pi$(arene)-ring interactions link molecules about inversion centres.

Related literature

For the biological activity of Schiff bases, see: Aydogan *et al.* (2001); Desai *et al.* (2001); El-masry *et al.* (2000); Hodnett & Dunn (1970); Kundu *et al.* (2005); Pandeya *et al.* (1999); Singh & Dash (1988); Taggi *et al.* (2002); Xu *et al.* (1997); For crystallography and coordination chemistry of compounds containing the azine functionality or a diimine linkage, see: Xu *et al.* (1997); Kundu *et al.* (2005); For related structures, see: Liu *et al.* (2007); Odabaşoğlu *et al.* (2007); Zhang & Zheng (2008); Zheng *et al.* (2005*a*,*b*). For standard bond lengths, see Allen *et al.* (1987).



Experimental

Crystal data

$C_{26}H_{20}N_2O_2$
M_r = 392.44
Monoclinic, $C2/c$
a = 23.6271 (16) Å
b = 11.2942 (6) Å
c = 8.2359 (7) Å
β = 109.538 (8)°
V = 2071.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 170 K
0.44 × 0.20 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.966, T_{max} = 0.995
4228 measured reflections
2341 independent reflections
1643 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.05
2341 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C7–C12 benzylidene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$A\cdots Cg^{i}$	0.93	2.68	3.5947 (17)	167

Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2067).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans 2*, pp. S1–19.
Aydogan, F., Ocal, N., Turgut, Z. & Yolacan, C. (2001). *Bull. Korean Chem. Soc.* **22**, 476–480.
Desai, S. B., Desai, P. B. & Desai, K. R. (2001). *Heterocycl. Commun.* **7**, 83–90.
El-masry, A. H., Fahmy, H. H. & Abdelwahed, S. H. A. (2000). *Molecules*, **5**, 1429–1438.
Hodnett, E. M. & Dunn, W. J. (1970). *J. Med. Chem.* **13**, 768–770.
Kundu, N., Chatterjee, P. B., Chaudhury, M. & Tiekink, E. R. T. (2005). *Acta Cryst.* E**61**, m1583–m1585.
Liu, G., Xie, L., Wang, Y. & Wang, J.-D. (2007). *Acta Cryst.* E**63**, o2611.
Odabaşoğlu, M., Büyükgüngör, O., Sunil, K. & Narayana, B. (2007). *Acta Cryst.* E**63**, o4145–o4146.
Oxford Diffraction (2010). *CrysAlis PRO* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
Pandeya, S. N., Sriram, D., Nath, G. & De Clercq, E. (1999). *Farmaco*, **54**, 624–628.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Singh, W. M. & Dash, B. C. (1988). *Pesticides*, **22**, 33–37.
Taggi, A. E., Hafez, A. M., Wack, H., Young, B., Ferraris, D. & Lectka, T. (2002). *J. Am. Chem. Soc.* **124**, 6626–6635.
Xu, Z., Thompson, L. K. & Miller, D. O. (1997). *Inorg. Chem.* **36**, 3985–3995.
Zhang, C.-N. & Zheng, Y.-F. (2008). *Acta Cryst.* E**64**, o36.
Zheng, P.-W., Wang, W. & Duan, X.-M. (2005*a*). *Acta Cryst.* E**61**, o3485–o3486.
Zheng, P.-W., Wang, W. & Duan, X.-M. (2005*b*). *Acta Cryst.* E**61**, o3020–o3021.

supporting information

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1,2-Bis(3-phenoxybenzylidene)hydrazine

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S1. Comment

Schiff bases are known to exhibit biological activity such as antimicrobial (El-masry *et al.*, 2000 & Pandeya *et al.*, 1999), antifungal (Singh & Dash, 1988), antitumor (Hodnett & Dunn, 1970; Desai *et al.*, 2001) and as herbicides. Moreover, Schiff bases are used as substrates in the preparation of number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Schiff bases have also been employed as ligands for complexation of metal ions (Aydogan *et al.*, 2001). On the industrial scale, they have wide range of applications such as dyes and pigments (Taggi *et al.*, 2002). Compounds containing an azine functionality or a diimine linkage have been investigated in terms of their crystallography and coordination chemistry (Xu *et al.*, 1997; Kundu *et al.*, 2005).

The crystal structures of some Schiff base hydrazines, *viz.*, 4-fluorobenzaldehyde[(E)-4-fluorobenzylidene]hydrazone (Odabaşoğlu *et al.*, 2007), N,N′-bis(3-nitrobenzylidene)hydrazine (Zheng *et al.*, 2005*a*), N,N′-Bis(4-chlorobenzylidene)hydrazine (Zheng *et al.*, 2005*b*), 1,2-bis(2-chlorobenzylidene)hydrazine (Zhang & Zheng, 2008), N,N′-Bis(4-hydroxybenzylidene)hydrazine (Liu *et al.*, 2007) have been reported. In view of the importance of Schiff base hydrazines, the crystal structure of title compound (I) is reported herein.

The complete molecule of the title compound, $C_{26}H_{20}N_2O_2$, is generated by the application of a centre of inversion (Fig. 1). The benzylidene ring is essentially coplanar with the central hydrazine group [dihedral angle = 4.5 (2)°] The dihedral angle between the mean plane of the 1,2-bis(benzylidene) hydrazine group and the two parallel phenyl rings is 34.0 (3)°. Weak C—H···Cg π-ring intermolecular interactions are observed (Table 1) providing some crystal packing stability (Fig. 2).

S2. Experimental

A mixture of 3-phenoxybenzaldehyde (0.02 mol) and hydrazine hydrate (0.012 mol) was refluxed in 15 ml of absolute alcohol containing 2 drops of sulfuric acid, for about 3 hours. On cooling, the resulting solid was filtered and dried. Single crystals were grown from DMF (dimethylformamide) by the slow evaporation method. Yield: 86%. (m.p.: 404 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.93Å (C–H). Isotropic displacement parameters for these atoms were set to 1.19-1.20 (CH) times U_{eq} of the parent atom.

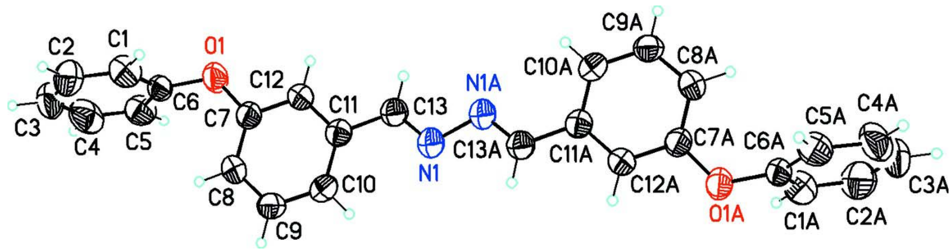

Figure 1

Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

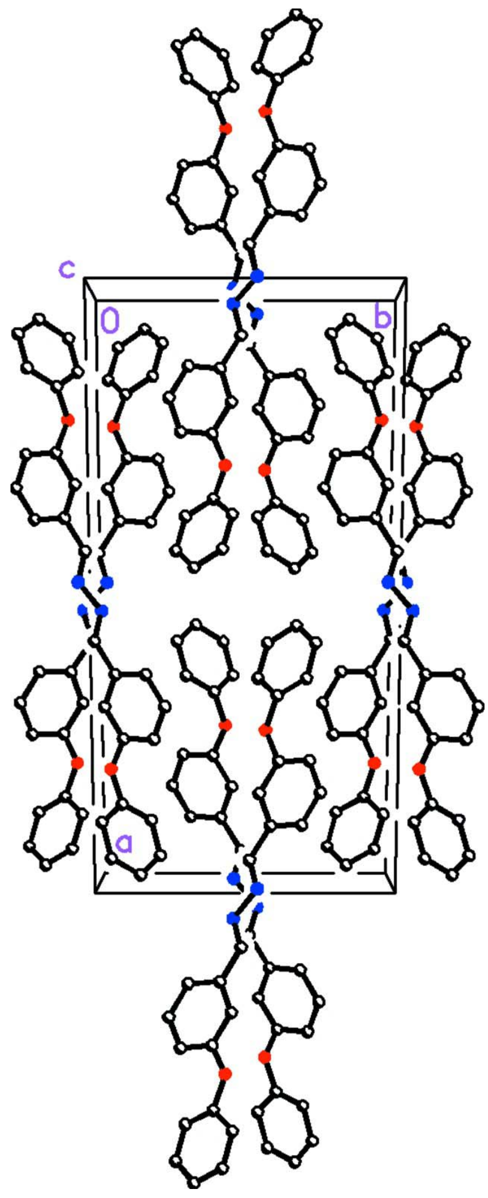

Figure 2

Packing diagram of the title compound viewed along the *c* axis. The H atoms have been removed for clarity.

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Crystal data

$C_{26}H_{20}N_2O_2$
$M_r = 392.44$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 23.6271$ (16) Å
$b = 11.2942$ (6) Å
$c = 8.2359$ (7) Å
$\beta = 109.538$ (8)°
$V = 2071.2$ (3) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.259$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1146 reflections
$\theta = 3.1$–28.6°
$\mu = 0.08$ mm^{-1}
$T = 170$ K
Plate, yellow
0.44 × 0.20 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1500 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
$T_{min} = 0.966$, $T_{max} = 0.995$
4228 measured reflections
2341 independent reflections
1643 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.7°$, $\theta_{min} = 3.1°$
$h = -31 \rightarrow 19$
$k = -12 \rightarrow 14$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.144$
$S = 1.05$
2341 reflections
136 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.4457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.28415 (5)	0.56492 (12)	0.14723 (17)	0.0634 (4)
N1	0.02329 (6)	0.53855 (12)	0.04610 (19)	0.0533 (4)
C1	0.36654 (9)	0.54126 (16)	0.4051 (2)	0.0582 (5)
H1B	0.3467	0.4787	0.4361	0.070*

C2	0.42338 (10)	0.5731 (2)	0.5077 (3)	0.0769 (7)
H2A	0.4421	0.5321	0.6096	0.092*
C3	0.45254 (9)	0.6644 (2)	0.4612 (3)	0.0818 (7)
H3A	0.4911	0.6854	0.5310	0.098*
C4	0.42510 (10)	0.7249 (2)	0.3120 (3)	0.0760 (7)
H4A	0.4450	0.7870	0.2802	0.091*
C5	0.36825 (9)	0.69433 (15)	0.2091 (2)	0.0584 (5)
H5A	0.3493	0.7355	0.1076	0.070*
C6	0.33985 (7)	0.60286 (14)	0.2574 (2)	0.0432 (4)
C7	0.23306 (7)	0.60721 (15)	0.1737 (2)	0.0442 (4)
C8	0.23209 (7)	0.70730 (14)	0.2691 (2)	0.0483 (4)
H8A	0.2672	0.7497	0.3218	0.058*
C9	0.17840 (8)	0.74360 (15)	0.2851 (2)	0.0491 (4)
H9A	0.1776	0.8111	0.3491	0.059*
C10	0.12623 (7)	0.68200 (14)	0.2084 (2)	0.0462 (4)
H10A	0.0905	0.7071	0.2213	0.055*
C11	0.12717 (7)	0.58123 (13)	0.1108 (2)	0.0416 (4)
C12	0.18101 (7)	0.54480 (14)	0.0936 (2)	0.0441 (4)
H12A	0.1820	0.4783	0.0281	0.053*
C13	0.07271 (7)	0.51346 (15)	0.0257 (2)	0.0469 (4)
H13A	0.0743	0.4504	−0.0452	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0376 (6)	0.0815 (9)	0.0687 (9)	−0.0038 (6)	0.0148 (6)	−0.0324 (7)
N1	0.0396 (8)	0.0516 (9)	0.0670 (10)	−0.0047 (6)	0.0156 (7)	−0.0052 (7)
C1	0.0663 (12)	0.0553 (11)	0.0548 (11)	−0.0063 (9)	0.0226 (9)	0.0036 (9)
C2	0.0680 (14)	0.0838 (16)	0.0605 (13)	0.0133 (13)	−0.0029 (11)	0.0005 (11)
C3	0.0425 (11)	0.0966 (18)	0.0949 (18)	−0.0106 (12)	0.0079 (11)	−0.0309 (15)
C4	0.0707 (14)	0.0690 (14)	0.0975 (18)	−0.0299 (12)	0.0403 (14)	−0.0178 (13)
C5	0.0670 (12)	0.0496 (10)	0.0595 (11)	−0.0038 (9)	0.0225 (10)	0.0045 (9)
C6	0.0354 (8)	0.0473 (9)	0.0479 (9)	−0.0026 (7)	0.0152 (7)	−0.0100 (7)
C7	0.0383 (8)	0.0501 (9)	0.0433 (9)	0.0021 (7)	0.0123 (7)	−0.0041 (7)
C8	0.0431 (9)	0.0499 (10)	0.0466 (9)	−0.0039 (8)	0.0080 (7)	−0.0081 (8)
C9	0.0516 (10)	0.0447 (9)	0.0482 (10)	0.0061 (8)	0.0131 (8)	−0.0054 (8)
C10	0.0434 (9)	0.0477 (9)	0.0479 (9)	0.0082 (7)	0.0157 (7)	0.0030 (7)
C11	0.0407 (8)	0.0412 (9)	0.0425 (9)	0.0005 (7)	0.0134 (7)	0.0047 (7)
C12	0.0423 (9)	0.0431 (9)	0.0459 (9)	−0.0014 (7)	0.0133 (7)	−0.0063 (7)
C13	0.0436 (9)	0.0453 (9)	0.0527 (10)	−0.0013 (7)	0.0175 (8)	−0.0007 (8)

Geometric parameters (Å, º)

O1—C7	1.3814 (18)	C5—H5A	0.9300
O1—C6	1.3930 (18)	C7—C12	1.379 (2)
N1—C13	1.266 (2)	C7—C8	1.381 (2)
N1—N1^{i}	1.410 (3)	C8—C9	1.381 (2)
C1—C6	1.359 (2)	C8—H8A	0.9300

C1—C2	1.374 (3)	C9—C10	1.372 (2)
C1—H1B	0.9300	C9—H9A	0.9300
C2—C3	1.364 (3)	C10—C11	1.398 (2)
C2—H2A	0.9300	C10—H10A	0.9300
C3—C4	1.365 (3)	C11—C12	1.388 (2)
C3—H3A	0.9300	C11—C13	1.459 (2)
C4—C5	1.371 (3)	C12—H12A	0.9300
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.362 (2)		

C7—O1—C6	118.43 (12)	C12—C7—O1	115.75 (14)
C13—N1—N1^{i}	112.25 (17)	C8—C7—O1	123.66 (14)
C6—C1—C2	118.82 (18)	C9—C8—C7	119.21 (15)
C6—C1—H1B	120.6	C9—C8—H8A	120.4
C2—C1—H1B	120.6	C7—C8—H8A	120.4
C3—C2—C1	120.4 (2)	C10—C9—C8	121.21 (15)
C3—C2—H2A	119.8	C10—C9—H9A	119.4
C1—C2—H2A	119.8	C8—C9—H9A	119.4
C2—C3—C4	119.92 (19)	C9—C10—C11	119.53 (15)
C2—C3—H3A	120.0	C9—C10—H10A	120.2
C4—C3—H3A	120.0	C11—C10—H10A	120.2
C3—C4—C5	120.2 (2)	C12—C11—C10	119.42 (14)
C3—C4—H4A	119.9	C12—C11—C13	119.11 (14)
C5—C4—H4A	119.9	C10—C11—C13	121.47 (14)
C6—C5—C4	119.14 (19)	C7—C12—C11	120.06 (15)
C6—C5—H5A	120.4	C7—C12—H12A	120.0
C4—C5—H5A	120.4	C11—C12—H12A	120.0
C1—C6—C5	121.55 (17)	N1—C13—C11	121.53 (15)
C1—C6—O1	118.67 (15)	N1—C13—H13A	119.2
C5—C6—O1	119.58 (16)	C11—C13—H13A	119.2
C12—C7—C8	120.56 (15)		

C6—C1—C2—C3	−0.5 (3)	O1—C7—C8—C9	178.76 (16)
C1—C2—C3—C4	0.2 (3)	C7—C8—C9—C10	0.1 (3)
C2—C3—C4—C5	0.1 (3)	C8—C9—C10—C11	−0.6 (2)
C3—C4—C5—C6	−0.2 (3)	C9—C10—C11—C12	0.3 (2)
C2—C1—C6—C5	0.4 (3)	C9—C10—C11—C13	−179.48 (15)
C2—C1—C6—O1	175.27 (16)	C8—C7—C12—C11	−1.1 (3)
C4—C5—C6—C1	0.0 (3)	O1—C7—C12—C11	−179.24 (14)
C4—C5—C6—O1	−174.87 (16)	C10—C11—C12—C7	0.5 (2)
C7—O1—C6—C1	88.2 (2)	C13—C11—C12—C7	−179.68 (14)
C7—O1—C6—C5	−96.80 (19)	N1^{i}—N1—C13—C11	−179.40 (15)
C6—O1—C7—C12	−163.42 (14)	C12—C11—C13—N1	175.49 (16)
C6—O1—C7—C8	18.5 (2)	C10—C11—C13—N1	−4.7 (3)
C12—C7—C8—C9	0.7 (3)		

Symmetry code: (i) $-x$, $-y$+1, $-z$.

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C7–C12 benzylidene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···*Cg*$^{\rm ii}$	0.93	2.68	3.5947 (17)	167

Symmetry code: (ii) $-x+1/2$, $-y+1/2$, $-z$.